

Ethane
74-84-0 | DTXSID6026377

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.42

Global applicability domain: Inside

Local applicability domain index: 5.59e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

Image not found

Ethane

Measured: 1.81

Predicted: 1.42

Image not found

Propane

Measured: 2.36

Predicted: 2.38

Image not found

1,2-Propylene oxide

Measured: 0.03

Predicted: 4.50e-02

Image not found

2-Propanol, 1,3-difluoro-

Measured: -0.360

Predicted: -0.0748

Image not found

1,2-Epoxy-3-fluoropropane

Measured: -0.160

Predicted: -0.152